Smirnite (Bi_2TeO_5) Structure: A2B5C_oC64_39_2cd_ac4d_d-001

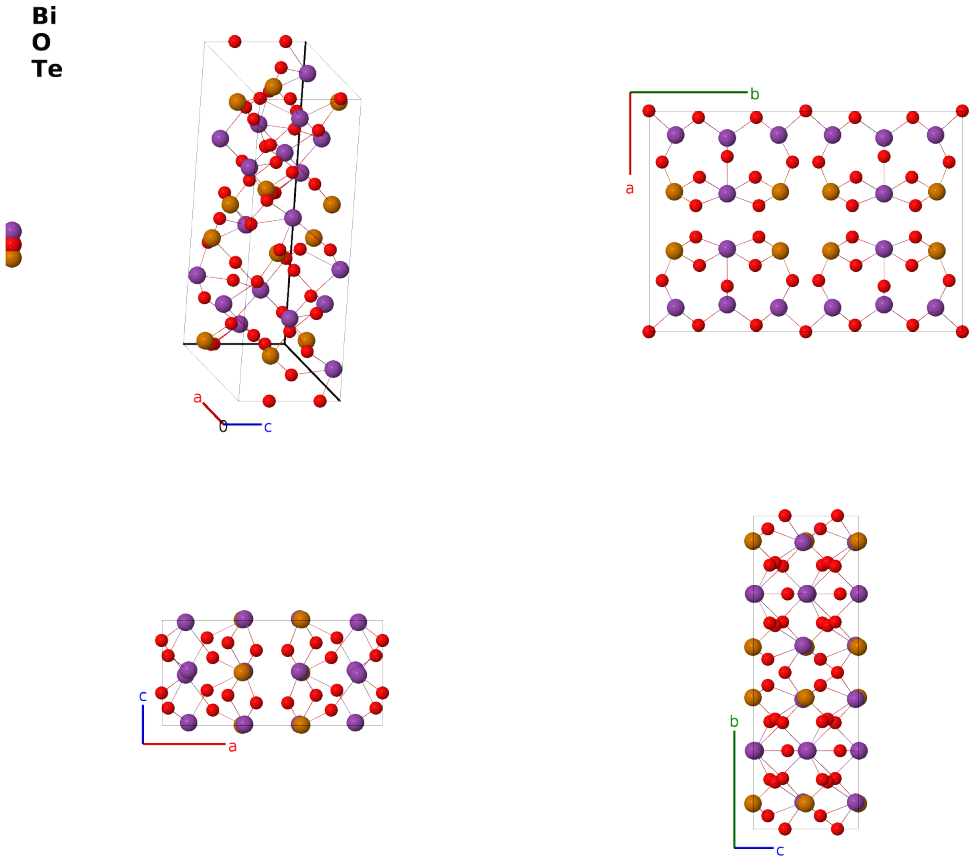
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/J44L

https://aflow.org/prototype-encyclopedia/A2B5C_oC64_39_2cd_ac4d_d-001



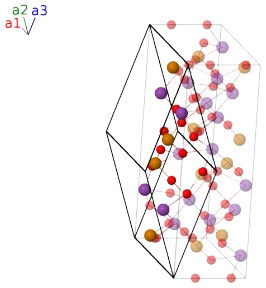
Prototype	Bi_2O_5Te
AFLOW prototype label	A2B5C_oC64_39_2cd_ac4d_d-001
Mineral name	smirnite
ICSD	36446
CCDC	1608173
Pearson symbol	oC64
Space group number	39
Space group symbol	$Aem2$

AFLOW prototype command `aflow --proto=A2B5C_oC64_39_2cd_ac4d_d-001 --params=`$a, b/a, c/a, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- Space group $Amb2$ #39 allows an arbitrary placement of the origin of the z-axis. Here $z_{10} = 0$ for the tellurium (8d) site.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$-\left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - \left(z_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(z_4 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Bi III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Bi III
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Bi III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Bi III
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 + (y_6 + z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - (y_6 - z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O III

$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1+(y_7-z_7)\,\mathbf{a}_2+(y_7+z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1-(y_7+z_7)\,\mathbf{a}_2-(y_7-z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1+\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{21}}$	=	$x_8\,\mathbf{a}_1+(y_8-z_8)\,\mathbf{a}_2+(y_8+z_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{22}}$	=	$-x_8\,\mathbf{a}_1-(y_8+z_8)\,\mathbf{a}_2-(y_8-z_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{23}}$	=	$x_8\,\mathbf{a}_1-\left(y_8+z_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{24}}$	=	$-x_8\,\mathbf{a}_1+\left(y_8-z_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{25}}$	=	$x_9\,\mathbf{a}_1+(y_9-z_9)\,\mathbf{a}_2+(y_9+z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{26}}$	=	$-x_9\,\mathbf{a}_1-(y_9+z_9)\,\mathbf{a}_2-(y_9-z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{27}}$	=	$x_9\,\mathbf{a}_1-\left(y_9+z_9-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{28}}$	=	$-x_9\,\mathbf{a}_1+\left(y_9-z_9+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{29}}$	=	$x_{10}\,\mathbf{a}_1+(y_{10}-z_{10})\,\mathbf{a}_2+(y_{10}+z_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_{30}}$	=	$-x_{10}\,\mathbf{a}_1-(y_{10}+z_{10})\,\mathbf{a}_2-(y_{10}-z_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_{31}}$	=	$x_{10}\,\mathbf{a}_1-\left(y_{10}+z_{10}-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_{32}}$	=	$-x_{10}\,\mathbf{a}_1+\left(y_{10}-z_{10}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	Te I

References

[1] D. Mercurio, M. E. Farissi, B. Frit, and P. Goursat, *Etude structurale et densification d'un nouveau materiau piezoelectrique: Bi_2TeO_5*, Mater. Chem. Phys. **9**, 467–476 (1983), doi:10.1016/0254-0584(83)90073-1.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).